Regularized BIE formulations for first- and second-order shape sensitivity of elastic fields[1]

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Abstract

The subject of this paper is the formulation of boundary integral equations for first- and second-order shape sensitivities of boundary elastic fields in three-dimensional bodies. Here the direct differentiation approach is considered. It relies on the repeated application of the material derivative concept to the governing regularized (i.e. weakly singular) displacement boundary integral equation (RDBIE) for an elastostatic state on a given domain. As a result, governing BIEs, which are also weakly singular, are obtained for the elastic sensitivities up to the second order. They are formulated so as to allow a straightforward implementation; in particular no strongly singular integral is involved. It is shown that the actual computation of shape sensitivities using usual BEM discretization uses the already built and factored discrete integral operators and needs only to set up additional right-hand sides and additional backsubstitutions. Some relevant discretization aspects are discussed.

1 Introduction

The consideration of first and second variations of integral functionals with respect to a geometrical domain arises in the study of many situations where a geometrical domain plays a major role. These include shape optimization processes with respect to mechanical constraints, usually expressed in terms of integrals involving the mechanical quantities (displacement, stress…) which themselves depend on the shape of the body. Geometrical inverse problems constitute a related area, where part of the domain boundary is unknown (e.g. in crack or defect identification), its determination being attempted by minimizing a distance between computed (for a given domain configuration) and known (for the actual, unknown, domain configuration) values of some mechanical quantity. Also, free-boundary problems can be dealt with using similar considerations. Finally, evolution problems in fracture or damage mechanics often involve geometrical fronts which propagate according to a Griffith-like criterion, where the second derivative of the potential energy at equilibrium with respect to front perturbations plays an essential role. All these situations share the common feature of involving integral functionals having both direct (through the geometrical support of the integral) and indirect (through mechanical fields which solve e.g. elastic boundary-value problems) dependence on the geometrical domain under consideration.

For many reasons (be it only computational efficiency), it is essential to be able to evaluate first and second variations of such functionals. Most usual optimization algorithms use first-order derivatives, while Newton-type algorithms also use second-order derivatives. Moreover, accurate evaluation of second-order derivatives may provide practical means of checking optimality conditions. Finally, as mentioned before, second-order derivatives of potential energy govern evolution problems involving energy release rates. Besides, it is also a known fact that finite-difference estimations of gradients (which would require here finite perturbations of the geometrical domain) are both computationally expensive and prone to inaccuracies due to the mathematically ill-posed nature of this problem. Hence it is natural to revert to analytical differentiation with respect to a variable domain. This concept has been studied and used by many authors (see e.g. Haug et al. [9], Petryk and Mroz [15]), up to now mainly in FEM-oriented contexts. However, since in such problems the domain (and hence its boundary) is a primary unknown, it is a natural idea to consider boundary integral formulations, because they offer in this context the “minimal” modelling.

The formulation of shape sensitivities, in a BIE context or otherwise, may result from the adjoint problem approach (APA) or the direct differentiation approach (DDA), applied either before and after discretization of the initial elastic BIE. Continuous formulations using the APA to shape sensitivity in a BIE context has been considered e.g. by Choi and Kwak [8] for 2D elasticity, Bonnet [3] for 3D geometrical inverse problems in acoustics, Burczinski and Fedelinski for transient elastodynamics [7], Meric [11] for thermal problems. The present paper deals with the analytical direct differentiation approach made at the continuous level. It consists in applying to the relevant governing BIE the material differentiation concept of continuum kinematics, the possibly non-material domain changes being described in terms of a finite number of parameters (e.g. design parameters in shape optimization) instead of the physical time variable. This leads to governing boundary integral equations for the shape sensitivities of elastic boundary variables. The latter may be considered for their own interest or as auxiliary variables which ultimately allow the computation of the shape sensitivities of domain- and state-dependent integral functionals. Other references about DDA include e.g. Nishimura and Kobayashi [14] for crack identification, Mukherjee and Chandra [12] for design sensitivities in nonlinear solid mechanics, Bonnet [4] for crack front stability, among others. A taylor series approach having some similarity with the DDA is given by Zeng and Saigal [20] for crack identification problems in potential theory. Also, the direct differentiation of discretized BEM formulations is treated in e.g. Kane et al. [10].

A difficulty with the DDA lies in the singular character of the governing BIE. Elastic BIE formulations were classically expressed in terms of Cauchy principal value (CPV) integrals. Barone and Yang [1] apply the material derivative concept to such CPV formulations. However, since the exclusion neighbourhood used in the limiting process which defines a CPV integral is distorted by a domain perturbation, this procedure raises the difficulty of whether the material derivative of a CPV integral equals the CPV of the material derivative of the integrand. The implicite answer to this is affirmative in [1], although in other instances erroneous results induced by misapplication of general techniques (change of variables, integration by parts…) to CPV integrals are well-known. Zhang and Mukherjee [21] circumvent this potential objection by using a 2D elastic BIE formulated in terms of tangential gradient of displacements ("derivative BIE") and thus of a weakly singular nature; they obtain weakly singular BIEs for first- and second-order elastic shape sensitivities. However, this kind of derivative BIE seems to be known only for 2D problems.

The present paper, of a theoretical nature, deals with BIE formulations for first- and second-order elastic shape sensitivities for 3D situations. To this end, the starting point is the regularized version of the conventional displacement BIE formulation (RDBIE), where only weakly singular integrals occur (see e.g. Rizzo and Shippy [16] for elastostatics, Bui et al. [6], Rizzo et al. [17] for steady-state elastodynamics, Bonnet [2] for transient elastodynamics). Applying the material derivatives to such formulations is mathematically sound, and results in weakly singular BIE formulations for first- and second-order shape sensitivities. The varying domains are mathematically described using diffeomorphisms between an "initial" configuration and the current one, using continuum kinematics approach. These diffeomorphisms depend on a finite number of parameters, so that all domain evolutions ultimately reduce to variations of those parameters. These parameters may either be actual design variables (for shape optimization) or result from the discretization of infinite-dimensional domain perturbations (e.g. crack front propagation in 3D fracture mechanics). This approach also allows to define and compute directional derivatives associated to any (sufficiently regular) boundary perturbation. As a result, first- and second- order shape sensitivities are defined in terms of transformation "velocities" and "accelerations", which are vector fields on the boundary.

The presentation here is restricted to 3D elastostatics for expository purposes but the analysis conducted extends to other situations as well: potential theory of course but also elastodynamics and acoustics. Firstly, some definitions are given regarding the material derivative concept, up to the second order, for functions and surface integrals; a short discussion of difficulties related to the definition of second-order domain derivatives is included. Then, starting from the RDBIE, the governing boundary integral equation for first-order shape sensitivity of an elastostatic state is established. The computation of first-order stress sensitivities at boundary points is then discussed. Next, the governing boundary integral equation for second-order shape sensitivity of an elastostatic state is derived. Finally, some relevant features of the BE discretization process are treated.

2 First- and second-order material derivative of a surface integral

Let us consider, in the three-dimensional Euclidean space $\mathbb{R}^3$ equipped with a Cartesian orthonormal basis $(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$, a body $\Omega_{\boldsymbol{p}}$ whose shape depends on a finite number of shape parameters $\boldsymbol{p} = (p_1, p_2, \ldots)$. The latter are treated as time-like parameters using a continuum kinematics-type lagrangian description and the "initial" configuration Ω_0 conventionally associated with $\boldsymbol{p} = \boldsymbol{0}$:

$$\boldsymbol{Y} \in \Omega_0 \rightarrow \boldsymbol{y} = \boldsymbol{\Phi}(\boldsymbol{Y}; \boldsymbol{p}) \in \Omega_{\boldsymbol{p}} \quad \text{where} \quad (\forall \boldsymbol{Y} \in \Omega_0) \;\; \boldsymbol{\Phi}(\boldsymbol{Y}; 0) = \boldsymbol{Y} \tag{1}$$

Throughout this paper lower-case boldface letters $\boldsymbol{x}, \boldsymbol{y}$ denote geometrical points on the current configuration $\Omega_{\boldsymbol{p}}$. The diffeomorphism $\boldsymbol{\Phi}(\cdot; \boldsymbol{p})$, or *geometrical transformation*, must possess a strictly positive Jacobian for any given $\boldsymbol{p}$. A given domain evolution considered as a whole, as is the case e.g. in shape optimization, admits many different representations (1), with different transformations $\boldsymbol{\Phi}$.

2.1 First-order material derivative

As far as first-order derivatives with respect to $\boldsymbol{p}$ are concerned, attention can be restricted to the consideration of a single parameter shape parameter p without loss of generality.

Material derivative of scalar or tensor fields. The *transformation velocity* $\boldsymbol{\theta}(\boldsymbol{y}; \boldsymbol{p})$, defined by

$$\boldsymbol{\theta}(\boldsymbol{y}; \boldsymbol{p}) = \boldsymbol{\Phi}_{,p}(\boldsymbol{Y}; \boldsymbol{p}) \qquad \text{for} \quad \boldsymbol{y} = \boldsymbol{\Phi}(\boldsymbol{Y}; \boldsymbol{p}) \tag{2}$$

is the (eulerian representation for the) "velocity" of the "material" point wich coincides with the geometrical point $\boldsymbol{y}$ at "time" p.

Next, let $f(\boldsymbol{y}; \boldsymbol{p})$ denote a scalar, vector or tensor field. The material derivative $\overset{\star}{f}(\boldsymbol{y}; \boldsymbol{p})$ in the domain transformation $\boldsymbol{y} = \boldsymbol{\Phi}(\boldsymbol{Y}; \boldsymbol{p})$ is defined (see e.g. Salençon [18]) as:

$$\begin{aligned} \overset{\star}{f}(\boldsymbol{y}; \boldsymbol{p}) &= g_{,p}(\boldsymbol{Y}; \boldsymbol{p}) \qquad \text{where} \quad g(\boldsymbol{Y}; \boldsymbol{p}) = f(\boldsymbol{\Phi}(\boldsymbol{Y}; \boldsymbol{p}); \boldsymbol{p}) \\ &= f_{,p}(\boldsymbol{y}; \boldsymbol{p}) + \boldsymbol{\nabla} f(\boldsymbol{y}; \boldsymbol{p}).\boldsymbol{\theta}(\boldsymbol{y}; \boldsymbol{p}) \end{aligned} \tag{3}$$

where $\boldsymbol{\nabla}$ denotes the gradient with respect to "eulerian" coordinates ($\boldsymbol{\nabla} f = (f_{,y_i}) \otimes \boldsymbol{e}_i$). The material derivative of the gradient $\boldsymbol{\nabla} f$ is thus given by:

$$\overset{\star}{\widehat{\nabla f}} = \boldsymbol{\nabla} \overset{\star}{f} - \boldsymbol{\nabla} f.\boldsymbol{\nabla}\boldsymbol{\theta} \tag{4}$$

while the material derivative of a *material* vector $\boldsymbol{a}$ attached to the moving point $\boldsymbol{y} = \boldsymbol{\Phi}(\boldsymbol{Y}; \boldsymbol{p})$ is given by:

$$\overset{\star}{\boldsymbol{a}} = \boldsymbol{\nabla}\boldsymbol{\theta}.\boldsymbol{a} \tag{5}$$

Material derivative of the surface differential element Let $S_{\boldsymbol{p}}$ be a material (in the sense of (1)) surface, and denote by $(\boldsymbol{a}, \boldsymbol{b})$ a pair of *material* vectors attached to a *material* point $\boldsymbol{y} = \boldsymbol{\Phi}(\boldsymbol{Y}; \boldsymbol{p})$, chosen so as to be unitary and orthogonal at a fixed value p_0 of p and to belong to the tangent plane at $\boldsymbol{y}$ to $S_{\boldsymbol{p}}$ for all p in a neighbourhood of p_0. For any such p, the unit normal to $S_{\boldsymbol{p}}$ at $\boldsymbol{y}$ is thus given by

$$\boldsymbol{n}(\boldsymbol{y}; \boldsymbol{p}) = \frac{1}{\parallel \boldsymbol{a} \wedge \boldsymbol{b} \parallel}(\boldsymbol{a} \wedge \boldsymbol{b})$$

Moreover, the surface differential element $\mathrm{d}S$ at $\boldsymbol{y}$ is proportional to the norm $\parallel \boldsymbol{a} \wedge \boldsymbol{b} \parallel$, so that:

$$\overset{\star}{\widehat{\mathrm{d}S}} = \parallel \boldsymbol{a} \wedge \boldsymbol{b} \parallel^{\star} \ \mathrm{d}S \tag{6}$$

The material derivative of the vector product $\boldsymbol{a} \wedge \boldsymbol{b}$ is then taken for the particular value p_0 of p, using (5):

$$\begin{aligned}
(\boldsymbol{a} \wedge \boldsymbol{b})^{\star} &= (\boldsymbol{\nabla}\boldsymbol{\theta}.\boldsymbol{a}) \wedge \boldsymbol{b} + \boldsymbol{a} \wedge (\boldsymbol{\nabla}\boldsymbol{\theta}.\boldsymbol{b}) \\
&= [(\boldsymbol{\nabla}\boldsymbol{\theta})_{aa} + (\boldsymbol{\nabla}\boldsymbol{\theta})_{bb}]\boldsymbol{n} - (\boldsymbol{\nabla}\boldsymbol{\theta})_{na}\boldsymbol{a} - (\boldsymbol{\nabla}\boldsymbol{\theta})_{nb}\boldsymbol{b} \\
&= (\mathrm{div}_S\boldsymbol{\theta})\boldsymbol{n} - \boldsymbol{n}.\boldsymbol{\nabla}_S\boldsymbol{\theta}
\end{aligned}$$

where the fact that $(\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{n})$ is an orthonormal vector frame at $p = p_0$ has been used. The surface gradient $\boldsymbol{\nabla}_S$ and divergence div_S are defined by:

$$\boldsymbol{\nabla}_S f = \boldsymbol{\nabla} f - (\boldsymbol{\nabla} f.\boldsymbol{n})\boldsymbol{n} = (f_{,i} - n_i f_{,n})\boldsymbol{e}_i \equiv (D_i f)\boldsymbol{e}_i \tag{7}$$

$$\mathrm{div}_S\boldsymbol{u} = \mathrm{div}\,\boldsymbol{u} - (\boldsymbol{\nabla}\boldsymbol{u}.\boldsymbol{n}).\boldsymbol{n} = D_i u_i \tag{8}$$

Moreover, one has:

$$\parallel \boldsymbol{a} \wedge \boldsymbol{b} \parallel^{\star} = \frac{\boldsymbol{a} \wedge \boldsymbol{b}}{\parallel \boldsymbol{a} \wedge \boldsymbol{b} \parallel}.(\boldsymbol{a} \wedge \boldsymbol{b})^{\star} = \boldsymbol{n}.(\boldsymbol{a} \wedge \boldsymbol{b})^{\star} = \mathrm{div}_S\boldsymbol{\theta}$$

As a result, the material derivatives of $\boldsymbol{n}$ and $\mathrm{d}S$ at $\boldsymbol{y} \in S_{\boldsymbol{p}}$ are given by:

$$\overset{\star}{\mathrm{d}S} = \mathrm{div}_S\boldsymbol{\theta}\,\mathrm{d}S = D_r\theta_r\,\mathrm{d}S \qquad \overset{\star}{\boldsymbol{n}} = -\boldsymbol{n}.\boldsymbol{\nabla}_S\boldsymbol{\theta} = -n_r D_j\theta_r\boldsymbol{e}_j \tag{9}$$

Material derivative of surface integrals The material derivative of an integral $J(p)$ over a varying surface:

$$J(p) = \int_{S_p} f(\boldsymbol{y}, p) dS_p$$

is given, using (9), by the following classical formula:

$$\frac{d}{dp}J(p) = \overset{\star}{J} = \int_{S_p} \left\{ \overset{\star}{f}\ \mathrm{d}S + f\ \overset{\star}{\widehat{\mathrm{d}S}} \right\} = \int_{S_p} \left\{ \overset{\star}{f} + f\mathrm{div}_S\boldsymbol{\theta} \right\} \mathrm{d}S \tag{10}$$

Indeed $\overset{\star}{J}$ could be expressed in several other ways (see Petryk and Mroz [15]), but the above formula serves the purpose of the present paper.

2.2 Second-order material derivative

In order to consider mixed second-order derivatives w.r.t. two design parameters, attention can be restricted to a generic pair p_1, p_2 of shape parameters without loss of generality. The transformation velocities $\boldsymbol{\theta}$ and $\boldsymbol{\mu}$, as given by (2) for $p = p_1$ and $p = p_2$ respectively, are introduced, together with the second transformation derivative $\boldsymbol{\chi}$:

$$\boldsymbol{\chi}(\boldsymbol{y};\boldsymbol{p}) = \boldsymbol{\Phi}_{,p_1p_2}(\boldsymbol{Y};\boldsymbol{p}) \qquad \text{for} \quad \boldsymbol{y} = \boldsymbol{\Phi}(\boldsymbol{Y};\boldsymbol{p}) \tag{11}$$

Moreover, the following property holds:

$$\boldsymbol{\chi}(\boldsymbol{y};\boldsymbol{p}) = \overset{\star}{\boldsymbol{\mu}}(\boldsymbol{y};\boldsymbol{p}) = \overset{\vee}{\boldsymbol{\theta}}(\boldsymbol{y};\boldsymbol{p}) \tag{12}$$

Let $f(\boldsymbol{y};\boldsymbol{p})$ be a sufficiently regular (scalar or tensor) field, then we denote by $\overset{\star}{f}, \overset{\vee}{f}$ the two distinct material derivatives of f w.r.t. p_1 and p_2 respectively and by $\overset{\star\vee}{f}$ the second-order material derivative:

$$\overset{\star\vee}{f}(\boldsymbol{y};\boldsymbol{p}) = g_{,p_1p_2}(\boldsymbol{Y};\boldsymbol{p}) \qquad g(\boldsymbol{Y};\boldsymbol{p}) = f(\boldsymbol{\Phi}(\boldsymbol{Y};\boldsymbol{p});\boldsymbol{p}) \tag{13}$$

With the above definition, the equality $\overset{\star\vee}{f} = (\overset{\star}{f})^{\vee} = (\overset{\vee}{f})^{\star}$ holds, so that $\overset{\star\vee}{f}$ results from two successive applications of (3).

Second-order material derivative of surface integrals. According to those definitions, the second-order material derivative of the surface integral

$$J(\boldsymbol{p}) = \int_{S_p} f(\boldsymbol{y};\boldsymbol{p})\,\mathrm{d}S$$

considered as a function of $\boldsymbol{p}$ results from a further application of formula (10) (w.r.t. p_2) to the material derivative $\overset{\star}{J}$ as given by (10):

$$\overset{\star\vee}{J}(\boldsymbol{p}) = (\overset{\star}{J})^{\vee}(\boldsymbol{p}) = (\overset{\vee}{J})^{\star}(\boldsymbol{p}) = \int_{S_p} \left[\overset{\star\vee}{f} + \overset{\star}{f}\,\mathrm{div}_S\boldsymbol{\mu} + \overset{\vee}{f}\mathrm{div}_S\boldsymbol{\theta} + f(\mathrm{div}_S\boldsymbol{\theta})^{\vee} + f\mathrm{div}_S\boldsymbol{\theta}\mathrm{div}_S\boldsymbol{\mu} \right] \mathrm{d}S \tag{14}$$

where $\overset{\vee}{\widehat{\mathrm{div}_S\boldsymbol{\theta}}}$ is given (formula (68) of Appendix A.2) by :

$$\overset{\vee}{\widehat{\mathrm{div}_S\boldsymbol{\theta}}} = \overset{\vee}{\widehat{D_r\theta_r}} = \mathrm{div}_S\boldsymbol{\chi} - \boldsymbol{\nabla}_S\boldsymbol{\theta} : \boldsymbol{\nabla}_S\boldsymbol{\mu} + (\boldsymbol{n}.\boldsymbol{\nabla}_S\boldsymbol{\theta}).(\boldsymbol{n}.\boldsymbol{\nabla}_S\boldsymbol{\mu}) \tag{15}$$

2.3 Comments about the concept of second-order material derivative

One has in fact to be very careful in defining a second-order material derivative. For example, one could find natural to consider the action of two *successive* domain transformations, each associated with a scalar shape paremeter p_1, p_2:

$$\boldsymbol{Y} \rightarrow \boldsymbol{z} = \boldsymbol{\Phi}(\boldsymbol{Y}, p_1) \rightarrow \boldsymbol{y} = \boldsymbol{\Psi}(\boldsymbol{z}, p_2)$$

with transformation velocities $\boldsymbol{\theta}, \boldsymbol{\mu}$ associated respectively to $\boldsymbol{\Phi}, \boldsymbol{\Psi}$ according to (2). Then, a differentiation in the transformation $\boldsymbol{\Phi}$ followed by a differentiation of the result in the transformation $\boldsymbol{\Psi}$ would in general give $\overset{\vee}{\boldsymbol{\theta}} \neq \overset{\star}{\boldsymbol{\mu}}$, $\overset{\star\vee}{f} \neq \overset{\vee\star}{f}$, $\overset{\star\vee}{J} \neq \overset{\vee\star}{J}$. Thus such approach, although natural-looking, could prove to be inadequate. This peculiarity is related to the fact that in general the compositions of two geometrical transformations do not commute:

$$\boldsymbol{\Psi}(\boldsymbol{\Phi}(\boldsymbol{Y}, p_1), p_2) \neq \boldsymbol{\Phi}(\boldsymbol{\Psi}(\boldsymbol{Y}, p_2), p_1)$$

The presentation adopted for the present work is unambiguous in this respect since it defines material derivatives using functions of a finite number of variables $\boldsymbol{p}$; it is design variable-oriented in that it allows to deal with second derivatives of integrals on domains depending simultaneously on a finite number of parameters (the design variables).

Material derivative vs. domain derivative In an alternative approach, mathematically more sophisticated, to the concept of shape sensitivity, the *domain derivative* DJ (Simon [19]) of a domain-dependent functional $J(\Omega)$ is introduced. In this framework, (small) perturbations $\boldsymbol{\theta}$ of the domain Ω itself are considered without reference to any finite set of parameters $\boldsymbol{p}$:

$$\boldsymbol{y} \in \Omega \rightarrow \boldsymbol{y} + \delta\boldsymbol{y} \in \Omega + \delta\Omega \qquad \delta\boldsymbol{y} = \boldsymbol{\theta}(\boldsymbol{y})$$

where $\boldsymbol{\theta}$ belong to an infinite-dimensional function space $\mathcal{V}$. Then DJ is the linear operator over $\boldsymbol{\theta}$ such that:

$$\langle DJ(\Omega), \boldsymbol{\theta} \rangle = J(\Omega + \boldsymbol{\theta}) - J(\Omega) + o(|\boldsymbol{\theta}|_{\mathcal{V}}) \tag{16}$$

Not surprisingly, it turns out that expression (10), which is established for surfaces moving according to (1), i.e. for surface integrals ultimately depending on a single parameter p, is identical for a small variation $\boldsymbol{\theta}$ of Ω to the directional derivative $\langle DJ(\Omega), \boldsymbol{\theta} \rangle$ of J:

$$J(\Omega + \boldsymbol{\theta} dp) - J(\Omega) = \overset{\star}{J}\, dp + o(|\boldsymbol{\theta}|_{\mathcal{V}})$$

However, the two approaches are somewhat divergent at the second-order level. The *second-order domain derivative* $D^2 J(\Omega)$ (Simon [19]), based on domain perturbations of the form:

$$\boldsymbol{y} \in \Omega \rightarrow \boldsymbol{y} + \boldsymbol{\theta}(\boldsymbol{y}) + \boldsymbol{\mu}(\boldsymbol{y})$$

is accordingly defined as a bilinear form over the functional arguments $\boldsymbol{\theta}, \boldsymbol{\mu}$ such that:

$$D^2 J(\Omega)(\boldsymbol{\theta}, \boldsymbol{\mu}) = J(\Omega + (\boldsymbol{\theta} + \boldsymbol{\mu})) - J(\Omega) - \overset{\star}{J}(\Omega; \boldsymbol{\theta}) - \overset{\vee}{J}(\Omega; \boldsymbol{\mu}) + o(|\boldsymbol{\theta}|^2_{\mathcal{V}}, |\boldsymbol{\mu}|^2_{\mathcal{V}}) \tag{17}$$

with $\boldsymbol{\theta}, \boldsymbol{\mu}$ small, according to the general definition of the second-order variation of a functional. In contrast, the present definition (14) relies on domain perturbations of the form:

$$\boldsymbol{y} \in \Omega_{\boldsymbol{p}} \rightarrow \boldsymbol{y} + \boldsymbol{\theta}(\boldsymbol{y}; \boldsymbol{p})\delta p_1 + \boldsymbol{\mu}(\boldsymbol{y}; \boldsymbol{p})\delta p_2 + \frac{1}{2}\boldsymbol{\chi}(\boldsymbol{y}; \boldsymbol{p})\delta p_1 \delta p_2$$

Hence the present second-order material derivative does not in general coincide with Simon's second domain derivative, except for the special case of transformations such that $\boldsymbol{\chi} = 0$. Also, note that since $\Omega + (\boldsymbol{\theta} + \boldsymbol{\mu}) \neq (\Omega + \boldsymbol{\theta}) + \boldsymbol{\mu})$, the definition (17) does not result from two successive first-order domain differentiations.

3 First- and second-order elastic shape sensitivity formulation

3.1 Governing regularized elastic BIE

Any elastostatic state on a given three-dimensional body Ω with zero body forces is governed by the following regularized displacement boundary integral equation (RDBIE) (see Rizzo and Shippy [16], Bui et al. [6]):

$$\kappa u_k(\boldsymbol{x}) + \int_{\partial\Omega} [u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})] n_j(\boldsymbol{y}) \Sigma^k_{ij}(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}S_y - \int_{\partial\Omega} t_i(\boldsymbol{y}) U^k_i(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}S_y \tag{18}$$

or, introducing for later convenience an abbreviated form:

$$I_1(\boldsymbol{x}, \boldsymbol{u}) - I_2(\boldsymbol{x}, \boldsymbol{t}) = 0 \tag{19}$$

in terms of the displacement field $\boldsymbol{u}$, the traction vector $\boldsymbol{t} = \boldsymbol{T}^n(\boldsymbol{u}) \equiv \boldsymbol{\sigma}(\boldsymbol{u}).\boldsymbol{n}$ associated with the elastic stress $\boldsymbol{\sigma}$, the Kelvin infinite-space fundamental displacement components

$$U^k_i(\boldsymbol{x}, \boldsymbol{y}) = -\frac{1}{16\pi\mu(1-\nu)r} \left[(3-4\nu)\delta_{ik} + r_{,i} r_{,k} \right] \tag{20}$$

created at $\boldsymbol{y} \in \mathbb{R}^3$ by a unit point force applied at $\boldsymbol{x}$ (the collocation point) along the $\boldsymbol{e}_k$-direction, the Kelvin elastic stress tensor

$$\Sigma^k_{ij}(\boldsymbol{x}, \boldsymbol{y}) = -\frac{1}{8\pi(1-\nu)r^2} \left[(1-2\nu)(\delta_{ik} r_{,j} + \delta_{sk} r_{,i} - \delta_{ij} r_{,k}) + 3 r_{,isk} \right] \tag{21}$$

Also, $r = \parallel \boldsymbol{y} - \boldsymbol{x} \parallel$ is the Euclidian distance between $\boldsymbol{y}, \boldsymbol{x}$, μ, ν are the shear modulus and the Poisson ratio, and $\kappa = 0$ (Ω bounded) or $\kappa = 1$ ($\mathbb{R}^3 - \Omega$ bounded); $()_{,i}$ denotes a partial derivative with respect to y_i. The Kelvin solutions possess the following well-known property:

$$U^k_i(\boldsymbol{x}, \boldsymbol{y}) = U^k_i(\boldsymbol{y} - \boldsymbol{x}) \qquad \Sigma^k_{ij}(\boldsymbol{x}, \boldsymbol{y}) = \Sigma^k_{ij}(\boldsymbol{y} - \boldsymbol{x}) \tag{22}$$

The RDBIE (18) holds for *any* collocation point $\boldsymbol{x} \in \mathbb{R}^3$. The pair of primary variables $(\boldsymbol{u}, \boldsymbol{t}) \mid_{\partial\Omega}$ is termed “elastostatic state on Ω” in the sequel. The mathematical validity of (19) rests upon a Hölder continuity requirement for the displacement $\boldsymbol{u}$ at $\boldsymbol{x}$:

$$\exists C > 0, \ \exists \alpha \in]0, 1] \quad \text{such that} \quad \parallel \boldsymbol{u}(\boldsymbol{y}) - \boldsymbol{u}(\boldsymbol{x}) \parallel \leq C \parallel \boldsymbol{y} - \boldsymbol{x} \parallel^\alpha \tag{23}$$

which ensures the effectiveness of the regularizing effect of the term $[\boldsymbol{u}(\boldsymbol{y}) - \boldsymbol{u}(\boldsymbol{x})]$ in (18) (or equivalently the existence of the CPV integral in the strongly singular version of (18)).

3.2 First-order sensitivity formulation

Elastic shape sensitivities. A small perturbation of the domain Ω_p associated to a small increment dp of a typical design parameter p induces a perturbation of the elastostatic state $(\boldsymbol{u}, \boldsymbol{t})$, which may be expressed in terms of the first-order material derivatives $\overset{\star}{\boldsymbol{u}}, \overset{\star}{\boldsymbol{t}}$:

$$\delta \boldsymbol{u} = \overset{\star}{\boldsymbol{u}} \, dp + o(dp) \qquad \delta \boldsymbol{t} = \overset{\star}{\boldsymbol{t}} \, dp + o(dp)$$

This idea is consistent with the present BIE framework: the boundary $\partial\Omega_{\boldsymbol{p}}$ of a material domain $\Omega_{\boldsymbol{p}}$ is itself material, hence $(\overset{\star}{\boldsymbol{u}},\overset{\star}{\boldsymbol{t}})\mid_{\partial\Omega_{\boldsymbol{p}}}$ are completely determined by the knowledge of $(\boldsymbol{u},\boldsymbol{t})\mid_{\partial\Omega_{\boldsymbol{p}+d\boldsymbol{p}}}$ for the neighbouring perturbed boundary configurations: the material derivatives $(\overset{\star}{\boldsymbol{u}},\overset{\star}{\boldsymbol{t}})\mid_{\partial\Omega_{\boldsymbol{p}}}$ are taken while "staying on the moving boundary". Since the RDBIE (19) holds for any elastostatic state defined on $\Omega_{\boldsymbol{p}}$ for any p, taking its material derivative using formula (10) leads to a governing equation for $(\overset{\star}{\boldsymbol{u}},\overset{\star}{\boldsymbol{t}})$.

This operation is now carried out, with the assumption that the collocation point $\boldsymbol{x}$ also follows the material transformation (1). First, a direct application of formula (10) to the integral operators I_1, I_2 gives :

$$
\begin{aligned}
\overset{\star}{I}_1(\boldsymbol{x}) &= I_1(\boldsymbol{x},\overset{\star}{\boldsymbol{u}}) + J_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta}) && (24)\\
\overset{\star}{I}_2(\boldsymbol{x},\boldsymbol{t}) &= I_2(\boldsymbol{x},\overset{\star}{\boldsymbol{t}}) + J_2(\boldsymbol{x},\boldsymbol{t};\boldsymbol{\theta}) && (25)
\end{aligned}
$$

with

$$
\begin{aligned}
J_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta}) &= \int_{\partial\Omega}[u_i(\boldsymbol{y})-u_i(\boldsymbol{x})]\left\{\overset{\star}{n}_j(\boldsymbol{y})\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y}) + n_j(\boldsymbol{y})\overset{\star}{\Sigma}{}^k_{ij}(\boldsymbol{x},\boldsymbol{y})\right\}\mathrm{d}S_y\\
&\quad+\int_{\partial\Omega}[u_i(\boldsymbol{y})-u_i(\boldsymbol{x})]\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y})n_j(\boldsymbol{y})D_r\theta_r(\boldsymbol{y})\,\mathrm{d}S_y && (26)\\
J_2(\boldsymbol{x},\boldsymbol{t};\boldsymbol{\theta}) &= \int_{\partial\Omega} t_i(\boldsymbol{y})\left\{\overset{\star}{U}{}^k_i(\boldsymbol{x},\boldsymbol{y}) + U^k_i(\boldsymbol{x},\boldsymbol{y})D_r\theta_r(\boldsymbol{y})\right\}\mathrm{d}S_y && (27)
\end{aligned}
$$

where, as a consequence of (22), the material derivatives of U^k_i, Σ^k_{ij} are given by :

$$
\overset{\star}{\Sigma}{}^k_{ij}(\boldsymbol{x},\boldsymbol{y}) = [\theta_r(\boldsymbol{y})\frac{\partial}{\partial y_r} + \theta_r(\boldsymbol{x})\frac{\partial}{\partial x_r}]\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y}) = [\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})]\Sigma^k_{ij,r}(\boldsymbol{x},\boldsymbol{y}) \tag{28}
$$

$$
\overset{\star}{U}{}^k_i(\boldsymbol{x},\boldsymbol{y}) = [\theta_r(\boldsymbol{y})\frac{\partial}{\partial y_r} + \theta_r(\boldsymbol{x})\frac{\partial}{\partial x_r}]U^k_i(\boldsymbol{x},\boldsymbol{y}) = [\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})]U^k_{i,r}(\boldsymbol{x},\boldsymbol{y}) \tag{29}
$$

Next, taking (28) together with identities (9) into account in (26), one obtains:

$$
\begin{aligned}
J_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta}) &= \int_{\partial\Omega}[u_i(\boldsymbol{y})-u_i(\boldsymbol{x})][\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})]n_j(\boldsymbol{y})\Sigma^k_{ij,r}(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}S_y\\
&\quad-\int_{\partial\Omega}[u_i(\boldsymbol{y})-u_i(\boldsymbol{x})]\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y})\left\{n_r(\boldsymbol{y})D_j\theta_r(\boldsymbol{y}) - n_j(\boldsymbol{y})D_r\theta_r(\boldsymbol{y})\right\}\mathrm{d}S_y\\
&= \int_{\partial\Omega}[u_i(\boldsymbol{y})-u_i(\boldsymbol{x})][\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})]n_j(\boldsymbol{y})\Sigma^k_{ij,r}(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}S_y\\
&\quad-\int_{\partial\Omega}[u_i(\boldsymbol{y})-u_i(\boldsymbol{x})]\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y})D_{rj}\theta_r(\boldsymbol{y})\,\mathrm{d}S_y && (30)
\end{aligned}
$$

where the tangential differential operator D_{rj} is defined as:

$$
D_{rj}f = n_rD_jf - n_jD_rf = n_rf_{,j} - n_jf_{,r} = e_{rsj}e_{abj}n_af_{,b} \tag{31}
$$

Once the assumption $\boldsymbol{u}\in C^{0,\alpha}$ is made, the mathematical validity of expression (30) for $J_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta})$ relies upon the following additional requirement:

$$
\exists C>0 \text{ such that } \parallel \boldsymbol{\theta}(y)-\boldsymbol{\theta}(x)\parallel \leq C\parallel \boldsymbol{y}-\boldsymbol{x}\parallel \tag{32}
$$

Note that (32) does not require $\boldsymbol{\theta}$ to be C^1-continuous at $\boldsymbol{x}$; for instance the appearance of an edge out of an initially smooth $\partial\Omega$ is allowed.

Finally, it is convenient to rearrange expression (30) for $J_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta})$ further. To this end, one notes the following variant of Stokes' formula:

$$\int_S D_{rj} f \,\mathrm{d}S = e_{rsj} \int_S e_{abj} n_a f_{,b} \,\mathrm{d}S = 0$$

which is valid for the case of a piecewise regular *closed* surface S and provided f is continuous at the edges of S, if any. Then the following integration by parts pattern holds:

$$\begin{aligned}
&\int_{\partial\Omega} [u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})][\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})] n_j(\boldsymbol{y}) \Sigma^k_{ij,r}(\boldsymbol{x},\boldsymbol{y}) \,\mathrm{d}S_y \\
&= \; -\int_{\partial\Omega} [u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})][\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})] \left\{ D_{rj}\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y}) + n_r(\boldsymbol{y})\Sigma^k_{ij,j}(\boldsymbol{x},\boldsymbol{y}) \right\} \,\mathrm{d}S_y \\
&= \; -\int_{\partial\Omega} [u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})][\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})] D_{rj}\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y}) \,\mathrm{d}S_y \\
&= \; \int_{\partial\Omega} D_{rj}\{[u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})][\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})]\} \Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y}) \,\mathrm{d}S_y
\end{aligned} \tag{33}$$

the differential operator D_{rj} being understood as acting on the variable $\boldsymbol{y}$. Use has been made of the equilibrium equation $\Sigma^k_{ij,j} = 0$ $(\boldsymbol{y} \neq \boldsymbol{x})$. Then, due to (33) and

$$D_{rj} \left\{ [u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})][\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})] \right\} - [u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})] D_{rj}\theta_r(\boldsymbol{y}) = [\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})] D_{rj} u_i(\boldsymbol{y})$$

one obtains an alternative expression for $J_1(\boldsymbol{x})$ as follows :

$$J_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta}) = \int_{\partial\Omega} [\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})] D_{rj} u_i(\boldsymbol{y}) \Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y}) \,\mathrm{d}S_y \tag{34}$$

which is more compact than, and should be used instead of, (30) in BE implementations.

First-order sensitivity formulation. The previous calculations lead to the main result of this section, which states that the material derivatives $\overset{\star}{\boldsymbol{u}}, \overset{\star}{\boldsymbol{t}}$ associated with any elastostatic state $(\boldsymbol{u},\boldsymbol{t})$ on $\Omega = \Omega_{\boldsymbol{p}}$ are governed by the following boundary integral equation ("(first-order) rate BIE"), in abbreviated form:

$$I_1(\boldsymbol{x},\overset{\star}{\boldsymbol{u}}) - I_2(\boldsymbol{x},\overset{\star}{\boldsymbol{t}}) = -J_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta}) + J_2(\boldsymbol{x},\boldsymbol{t};\boldsymbol{\theta}) \tag{35}$$

where J_1, J_2 are given by eqns. (34), (27). This result holds for any collocation point $\boldsymbol{x} \in \mathbb{R}^3$, hence it defines an integral equation (if $\boldsymbol{x}$ is chosen on the boundary $\partial\Omega_{\boldsymbol{p}}$) or an integral representation of $\overset{\star}{\boldsymbol{u}}\,(\boldsymbol{x};\boldsymbol{p})$ (if $\boldsymbol{x}$ is chosen interior to $\Omega_{\boldsymbol{p}}$). Its right-hand side is an explicit linear expression of the transformation velocity $\boldsymbol{\theta}$. The BIE (35) is weakly singular provided $\boldsymbol{u}$ and $\boldsymbol{\theta}$ meet the requirements (23), (32) respectively. This is also true for all intermediate calculations used for the derivation of (35).

3.3 Shape sensitivity of stress at a regular boundary point

Using (4), one has:

$$\overset{\star}{\boldsymbol{\sigma}}\,(\boldsymbol{u}) = (\boldsymbol{C} : \boldsymbol{\nabla}\boldsymbol{u})^\star = \boldsymbol{\sigma}(\overset{\star}{\boldsymbol{u}}) - \boldsymbol{C} : (\nabla\boldsymbol{u}.\nabla\boldsymbol{\theta}) \tag{36}$$

where $C_{abcd} = \mu[\gamma\delta_{ab}\delta_{cd} + \delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc}]$ are the coefficients of Hooke's elastic tensor $(\gamma = 2\nu/(1-2\nu))$. One approach for the evaluation of $\overset{\star}{\boldsymbol{\sigma}}$, along the lines given in [21] for 2D problems, needs that of $\boldsymbol{\nabla}\boldsymbol{u}$

and $\boldsymbol{\nabla} \overset{\star}{\boldsymbol{u}}$ in terms of the boundary variables $\boldsymbol{u}, \boldsymbol{t}, \overset{\star}{\boldsymbol{u}}, \overset{\star}{\boldsymbol{t}}$. To this end one makes use of the decomposition $\boldsymbol{\nabla v} = \boldsymbol{\nabla}_S \boldsymbol{v} + \boldsymbol{v}_{,n} \otimes \boldsymbol{n}$ and is left to express $\boldsymbol{u}_{,n}, \overset{\star}{\boldsymbol{u}}_{,n}$ in terms of $\boldsymbol{t}, \overset{\star}{\boldsymbol{t}}$. First

$$\begin{aligned}\boldsymbol{t} &= \mu \left[\frac{2\nu}{1-2\nu} (\operatorname{div} \boldsymbol{u}) \boldsymbol{n} + \boldsymbol{u}_{,n} + \boldsymbol{n}.\boldsymbol{\nabla u} \right] \\ &= \mu \left[\frac{2\nu}{1-2\nu} (\operatorname{div}_S \boldsymbol{u}) \boldsymbol{n} + \boldsymbol{n}.\boldsymbol{\nabla}_S \boldsymbol{u} + \left(\frac{1}{1-2\nu} \boldsymbol{n} \otimes \boldsymbol{n} + \boldsymbol{I} \right) .\boldsymbol{u}_n \right]\end{aligned}$$

which can be inverted to yield:

$$\boldsymbol{u}_{,n} = \frac{1}{\mu} \left[\boldsymbol{I} - \frac{1}{2(1-\nu)} \boldsymbol{n} \otimes \boldsymbol{n} \right] .\boldsymbol{t} - \boldsymbol{n}.\boldsymbol{\nabla}_S \boldsymbol{u} - \frac{\nu}{1-\nu} (\operatorname{div}_S \boldsymbol{u}) \boldsymbol{n} \tag{37}$$

At this stage, the complete tensors $\boldsymbol{\nabla u}(\boldsymbol{x})$ and $\boldsymbol{\sigma}(\boldsymbol{x})$ are accessible from boundary data $\boldsymbol{u}, \boldsymbol{t}$.

Next, the material derivative $\overset{\star}{\boldsymbol{n}}$ (9) can be reformulated using eqns. (7-8) as:

$$\overset{\star}{\boldsymbol{n}} = (\boldsymbol{n}.\boldsymbol{\theta}_{,n}) \boldsymbol{n} - \boldsymbol{n}.\nabla \boldsymbol{\theta} = (\operatorname{div} \boldsymbol{\theta} - \operatorname{div}_S \boldsymbol{\theta}) \boldsymbol{n} - \boldsymbol{n}.\boldsymbol{\nabla \theta}$$

This, combined with (36), gives the following relationship

$$\overset{\star}{\boldsymbol{t}} = \overset{\star}{\widehat{\boldsymbol{\sigma}(\boldsymbol{u}).\boldsymbol{n}}} = \boldsymbol{T}^n(\overset{\star}{\boldsymbol{u}}) - \boldsymbol{A}.\boldsymbol{n} - (\operatorname{div}_S \boldsymbol{\theta}) \boldsymbol{t} \tag{38}$$

where

$$\boldsymbol{A} = \boldsymbol{C} : (\boldsymbol{\nabla u}.\boldsymbol{\nabla \theta}) - \boldsymbol{\sigma}(\boldsymbol{u}) \operatorname{div} \boldsymbol{\theta} + \boldsymbol{\sigma}(\boldsymbol{u}).(\boldsymbol{\nabla \theta})^T \tag{39}$$

Finally, one notices that identity (37) also holds for $\boldsymbol{u}, \boldsymbol{t}$ replaced with $\overset{\star}{\boldsymbol{u}}, \boldsymbol{T}^n(\overset{\star}{\boldsymbol{u}})$. This fact together with eqn. (38) yields the expression of $\overset{\star}{\boldsymbol{u}}_{,n}$ in terms of $\boldsymbol{\nabla}_S \overset{\star}{\boldsymbol{u}}, \overset{\star}{\boldsymbol{t}}$, which in turn gives $\boldsymbol{\nabla} \overset{\star}{\boldsymbol{u}}$ in terms of the boundary variables $\boldsymbol{\nabla}_S \overset{\star}{\boldsymbol{u}}, \overset{\star}{\boldsymbol{t}}$. Equation (36) is then applicable to compute the sensitivity of stress once the elastic and rate BIEs are solved.

Material differentiation of the stress boundary integral representation An alternative approach is to start from the regularized integral representation of $\boldsymbol{\nabla u}(\boldsymbol{x})$, which reads (Bonnet and Bui [5]):

$$\begin{aligned}(\frac{1}{2} - \kappa) u_{i,k}(\boldsymbol{x}) \quad &= \quad \int_{\partial\Omega} \left\{ [D_{rj} u_i(\boldsymbol{y}) - D_{rj} u_i(\boldsymbol{x})] \, \Sigma_{ij}^k(\boldsymbol{x}, \boldsymbol{y}) - [t_i(\boldsymbol{y}) - t_i(\boldsymbol{x})] \, U_{i,r}^k(\boldsymbol{x}, \boldsymbol{y}) \right\} \, \mathrm{d}S_y \\ &\quad + D_{rj} u_i(\boldsymbol{x}) A_{ij}^k(\boldsymbol{x}, \partial\Omega) - t_i(\boldsymbol{x}) B_{ir}^k(\boldsymbol{x}, \partial\Omega)\end{aligned} \tag{40}$$

where $A_{ij}^k(\boldsymbol{x}, \partial\Omega), B_{ir}^k(\boldsymbol{x}, \partial\Omega)$ denote regularized expressions for the integrals of $U_{i,r}^k, \Sigma_{ij}^k$ over $\partial\Omega$:

$$\begin{aligned}A_{ij}^k(\boldsymbol{x}, \partial\Omega) &= -\frac{1}{8\pi(1-\nu)} \left[(1-2\nu)[\delta_{ik} I_j(\boldsymbol{x}, \partial\Omega) + \delta_{sk} I_i(\boldsymbol{x}, \partial\Omega) - \delta_{ij} I_k(\boldsymbol{x}, \partial\Omega)] + J_{ijk}(\boldsymbol{x}, \partial\Omega) \right] \\ B_{ir}^k(\boldsymbol{x}, \partial\Omega) &= -\frac{1}{16\pi\mu(1-\nu)} \left[(3-4\nu) \delta_{ik} I_r(\boldsymbol{x}, \partial\Omega) + J_{ikr}(\boldsymbol{x}, \partial\Omega) - \delta_{rk} I_i(\boldsymbol{x}, \partial\Omega) - \delta_{ir} I_k(\boldsymbol{x}, \partial\Omega) \right]\end{aligned}$$

with

$$\begin{aligned}I_a(\boldsymbol{x}, \partial\Omega) &= \int_{\partial\Omega} \left(\frac{1}{r} r_{,n} - D_q n_q \right) n_a \frac{\mathrm{d}S}{r} \\ J_{abc}(\boldsymbol{x}, \partial\Omega) &= \delta_{ac} I_b(\boldsymbol{x}, \partial\Omega) + \delta_{bc} I_a(\boldsymbol{x}, \partial\Omega) + \int_{\partial\Omega} (r_{,b} r_{,q} D_{qa} n_c - D_a(n_b n_c) - D_b(n_a n_c)) \frac{\mathrm{d}S}{r} \\ &\quad + \int_{\partial\Omega} (2 n_a n_b - r_{,a} r_{,b}) n_c D_q n_q \frac{\mathrm{d}S}{r} + \int_{\partial\Omega} n_c r_{,n} (\delta_{ab} - 2 n_a n_b) \frac{\mathrm{d}S}{r^2}\end{aligned}$$

Then a crucial step for the evaluation of $\overset{\star}{\boldsymbol{\sigma}}$ as given by (36) is a material differentiation of the representation formula (40). This operation does not raise any conceptual difficulty, all the integrals being weakly singular. However, the derivation is somewhat tedious and the numerical evaluation of the resulting lengthy expression is expected to be time-consuming. At the same time, it is not clear whether this procedure leads to an improvement of accuracy for the stress sensitivity evaluation at boundary points, compared to the simpler method outlined in eqns. (37) to (39). This approach is developed in [1] but starting from a strongly singular version of (40).

3.4 Interpretation of the rate BIE as an elasticity problem

Let expression (38) for $\overset{\star}{\boldsymbol{t}}$ be inserted into the derivative $\overset{\star}{I}_2$, eqn. (25), which gives:

$$\begin{aligned} \overset{\star}{I}_2\,(\boldsymbol{x},\boldsymbol{t};\boldsymbol{\theta}) = &\int_{\partial\Omega} [\boldsymbol{T}^n(\overset{\star}{\boldsymbol{u}})]_i(\boldsymbol{y}) U_i^k(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}S_y \\ &+ \int_{\partial\Omega} \left\{ t_i(\boldsymbol{y})[\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})]U_{i,r}^k(\boldsymbol{x},\boldsymbol{y}) - A_{ij}(\boldsymbol{y})n_j(\boldsymbol{y})U_i^k(\boldsymbol{x},\boldsymbol{y})\right\}\,\mathrm{d}S_y \end{aligned} \tag{41}$$

where the $A_{ij}(\boldsymbol{y})$ are the coefficients of the tensor $\boldsymbol{A}$ defined by (39). Then an analytical transformation, given in the Appendix A.1, shows that:

$$\begin{aligned} &\int_{\partial\Omega} A_{ij}(\boldsymbol{y})n_j(\boldsymbol{y})U_i^k(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}S_y \\ &= \int_{\Omega} U_i^k(\boldsymbol{x},\boldsymbol{y})A_{ij,j}(\boldsymbol{y})\,\mathrm{d}V_y + \int_{\partial\Omega} t_i(\boldsymbol{y})[\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})]U_{i,r}^k(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}S_y \\ &\quad - \int_{\partial\Omega} [\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})]\Sigma_{ij}^k(\boldsymbol{x},\boldsymbol{y})D_{rj}u_i(\boldsymbol{y})\,\mathrm{d}S_y \end{aligned} \tag{42}$$

On account of the last two equations, the rate BIE (35) can be reformulated as a RDBIE on the boundary variables $\overset{\star}{\boldsymbol{u}}, \boldsymbol{T}^n(\overset{\star}{\boldsymbol{u}}))$ considered as an elastostatic state with nonzero body forces per unit volume given by $\boldsymbol{F}(\boldsymbol{y}) = -\mathrm{div}\,\boldsymbol{A}(\boldsymbol{y})$:

$$I_2(\boldsymbol{x},\boldsymbol{T}^n(\overset{\star}{\boldsymbol{u}})) - I_1(\boldsymbol{x},\overset{\star}{\boldsymbol{u}}) = -\int_{\Omega} U_i^k(\boldsymbol{x},\boldsymbol{y})A_{ij,j}(\boldsymbol{y})\,\mathrm{d}V_y \tag{43}$$

This result gives some understanding about the nature and structure of the rate BIE (35). Its right-hand side is seen to be related to a domain integral of the body-force kind (and more precisely of the initial-stress kind) which, in this particular instance, is analytically convertible into boundary integrals. More generally, the BIE (35) is related to an elastostatic boundary-value problem. This could have been shown using different means, e.g. a material derivative of a displacement-based variational formulation for the elasticity problem.

3.5 Second-order sensitivity formulation

The governing BIE over the second-order shape sensitivities of an elastostatic state is sought as the result of two successive application of the material derivative (with respect first to p_1, then to p_2) to the elastic RDBIE (19). This reduces to taking the material derivative w.r.t. p_2 of the first-order rate BIE (35), which holds true for any domain $\Omega_{\boldsymbol{p}}$, any elastostatic state $(\boldsymbol{u},\boldsymbol{t})$ and any first-order sensitivity pair $(\overset{\star}{\boldsymbol{u}},\overset{\star}{\boldsymbol{t}})$ on $\Omega_{\boldsymbol{p}}$.

Material derivative of the left-hand side of (35). The formal derivation used in the previous section to establish (35) from (19) is applicable to this step without modification except for the replacement of $(\boldsymbol{u},\boldsymbol{t})$ with $(\overset{\star}{\boldsymbol{u}},\overset{\star}{\boldsymbol{t}})$, and gives as a result:

$$\Big\{I_1(\boldsymbol{x},\overset{\star}{\boldsymbol{u}})-I_2(\boldsymbol{x},\overset{\star}{\boldsymbol{t}})\Big\}^{\vee}=I_1(\boldsymbol{x},\overset{\star\vee}{\boldsymbol{u}})+J_1(\boldsymbol{x},\overset{\star}{\boldsymbol{u}};\boldsymbol{\mu})-I_2(\boldsymbol{x},\overset{\star\vee}{\boldsymbol{t}})-J_2(\boldsymbol{x},\overset{\star}{\boldsymbol{t}};\boldsymbol{\mu}) \tag{44}$$

Material derivative of the right-hand side of (35). Application of formula (10) to $J_2(\boldsymbol{x},\boldsymbol{t};\boldsymbol{\theta})$ given by (27) gives, taking into account identity (15) :

$$\overset{\vee}{J}_2(\boldsymbol{x},\boldsymbol{t};\boldsymbol{\theta})=J_2(\boldsymbol{x},\overset{\vee}{\boldsymbol{t}};\boldsymbol{\theta})+J_2(\boldsymbol{x},\boldsymbol{t};\boldsymbol{\chi})+K_2(\boldsymbol{x},\boldsymbol{t};\boldsymbol{\theta},\boldsymbol{\mu}) \tag{45}$$

where

$$\begin{aligned}K_2(\boldsymbol{x},\boldsymbol{t};\boldsymbol{\theta},\boldsymbol{\mu}) \;&=\; \int_{\partial\Omega} t_i(\boldsymbol{y})U^k_{i,qr}(\boldsymbol{x},\boldsymbol{y})[\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})][\mu_q(\boldsymbol{y})-\mu_q(\boldsymbol{x})]\,\mathrm{d}S_y\\ &\quad+\int_{\partial\Omega} t_i(\boldsymbol{y})U^k_{i,r}(\boldsymbol{x},\boldsymbol{y})\left\{[\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})]D_q\mu_q(\boldsymbol{y})+[\mu_r(\boldsymbol{y})-\mu_r(\boldsymbol{x})]D_q\theta_q(\boldsymbol{y})\right\}\,\mathrm{d}S_y\\ &\quad+\int_{\partial\Omega} t_i(\boldsymbol{y})U^k_{i}(\boldsymbol{x},\boldsymbol{y})\left\{n_pn_rD_q\mu_pD_q\theta_r-D_r\mu_qD_q\theta_r+D_r\theta_rD_q\mu_q\right\}(\boldsymbol{y})\,\mathrm{d}S_y\end{aligned} \tag{46}$$

Likewise, the material derivative of integral $J_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta})$ is given by :

$$\begin{aligned}\overset{\vee}{J}_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta})=J_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\chi})&+\int_{\partial\Omega}[\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})]\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y})\{\overset{\vee}{\widehat{D_{rj}u_i}}(\boldsymbol{y})+D_{rj}u_i(\boldsymbol{y})D_q\mu_q(\boldsymbol{y})\}\,\mathrm{d}S_y\\ &+\int_{\partial\Omega}[\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})][\mu_q(\boldsymbol{y})-\mu_q(\boldsymbol{x})]\Sigma^k_{ij,q}(\boldsymbol{x},\boldsymbol{y})D_{rj}u_i(\boldsymbol{y})\,\mathrm{d}S_y\end{aligned}$$

Using eqn. (66) of Appendix A.2 for $\overset{\vee}{\widehat{D_{rj}u_i}}$, one obtains :

$$\overset{\vee}{J}_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta})=J_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\chi})+J_1(\boldsymbol{x},\overset{\vee}{\boldsymbol{u}};\boldsymbol{\theta})+K_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta},\boldsymbol{\mu}) \tag{47}$$

where

$$\begin{aligned}K_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta},\boldsymbol{\mu}) \;&=\; \int_{\partial\Omega}[\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})]\left\{[\mu_q(\boldsymbol{y})-\mu_q(\boldsymbol{x})]\Sigma^k_{ij,q}(\boldsymbol{x},\boldsymbol{y})+D_q\mu_q(\boldsymbol{y})\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y})\right\}D_{rj}u_i(\boldsymbol{y})\,\mathrm{d}S_y\\ &\quad+\int_{\partial\Omega}[\theta_r(\boldsymbol{y})-\theta_r(\boldsymbol{x})]\left\{D_j\mu_q(\boldsymbol{y})D_{qr}u_i(\boldsymbol{y})+D_r\mu_q(\boldsymbol{y})D_{sq}u_i(\boldsymbol{y})\right\}\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}S_y\end{aligned} \tag{48}$$

Second-order shape sensitivity formulation. The previous derivations lead to the main result of this section, which states that the second-order material derivatives $(\overset{\star\vee}{\boldsymbol{u}},\overset{\star\vee}{\boldsymbol{t}})$ associated with any geometrical transformation $\boldsymbol{\Phi}(\cdot;\boldsymbol{p})$ and any elastostatic state $\boldsymbol{u},\boldsymbol{t}$ on the domain $\Omega=\Omega_{\boldsymbol{p}}$ are governed by the following boundary integral equation ("second-order rate BIE"):

$$\begin{aligned}I_1(\boldsymbol{x},\overset{\star\vee}{\boldsymbol{u}})-I_2(\boldsymbol{x},\overset{\star\vee}{\boldsymbol{t}}) \;&=\; J_2(\boldsymbol{x},\overset{\star}{\boldsymbol{t}};\boldsymbol{\mu})+J_2(\boldsymbol{x},\overset{\vee}{\boldsymbol{t}};\boldsymbol{\theta})-J_1(\boldsymbol{x},\overset{\star}{\boldsymbol{u}};\boldsymbol{\mu})-J_1(\boldsymbol{x},\overset{\vee}{\boldsymbol{u}};\boldsymbol{\theta})\\ &\quad+J_2(\boldsymbol{x},\boldsymbol{t};\boldsymbol{\chi})-J_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\chi})+K_2(\boldsymbol{x},\boldsymbol{t};\boldsymbol{\theta},\boldsymbol{\mu})-K_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta},\boldsymbol{\mu})\end{aligned} \tag{49}$$

where J_1,J_2,K_1,K_2 are given by eqns. (34), (27), (46) and (48) respectively. This result holds true for any collocation point $\boldsymbol{x}\in\mathbb{R}^3$, hence it defines an integral equation (if $\boldsymbol{x}$ is chosen on the boundary $\partial\Omega_{\boldsymbol{p}}$) or an integral representation of $\overset{\star\vee}{\boldsymbol{u}}(\boldsymbol{x};\boldsymbol{p})$ (if $\boldsymbol{x}$ is chosen interior to $\Omega_{\boldsymbol{p}}$). The BIE (49) is weakly singular provided $\boldsymbol{u}$ and the pair $(\boldsymbol{\theta},\boldsymbol{\mu})$ meet the requirements (23), (32) respectively. This is also true for all intermediate steps used for the derivation of (49).

Symmetry of the second-order rate BIE. The right-hand side of (49) is symmetric with respect to $(\boldsymbol{\theta},\boldsymbol{\mu})$, due to what follows. First, the symmetric character w.r.t. $(\boldsymbol{\theta},\boldsymbol{\mu})$ of $J_2(\boldsymbol{x},\overset{\vee}{\boldsymbol{t}};\boldsymbol{\theta}) + J_2(\boldsymbol{x},\overset{\star}{\boldsymbol{t}};\boldsymbol{\mu}) - J_1(\boldsymbol{x},\overset{\star}{\boldsymbol{u}};\boldsymbol{\mu}) - J_1(\boldsymbol{x},\overset{\vee}{\boldsymbol{u}};\boldsymbol{\theta})$ is clearly visible from eqns. (34-27). Then $K_2(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta},\boldsymbol{\mu})$ is also symmetric in view of eqn. (46). Next, the symmetric character w.r.t. $(\boldsymbol{\theta},\boldsymbol{\mu})$ of $J_2(\boldsymbol{x},\boldsymbol{t};\boldsymbol{\chi}) - J_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\chi})$ stems from the property (12) of $\boldsymbol{\chi}$. Finally, the symmetric character of $K_1(\boldsymbol{x},\boldsymbol{u};\boldsymbol{\theta},\boldsymbol{\mu})$, which is not apparent in eqn. (48), is established in Appendix A.3.

It is worth mentioning that such symmetry considerations are of primary importance in contexts such as stability/bifurcation analysis of e.g. crack fronts using second-order shape sensitivities (see e.g. Nguyen [13]).

3.6 Comments about the sensitivity BIE formulations

The first-order rate BIE (35) does not define, for a given transformation velocity $\boldsymbol{\theta}$, a unique pair $(\overset{\star}{\boldsymbol{u}},\overset{\star}{\boldsymbol{t}})$. In order to do so, one has in addition to specify how the boundary conditions associated with the elastic problem evolve with $\Omega_{\boldsymbol{p}}$. It is simplest to assume that the transformation $\boldsymbol{\Phi}(\cdot;\boldsymbol{p})$ which describes a given change of domain is chosen so that (say) the Dirichlet and Neumann parts of $\partial\Omega_{\boldsymbol{p}}$ are respectively transformed into the Dirichlet and Neumann parts of $\partial\Omega_{\boldsymbol{p}+d\boldsymbol{p}}$, in which case $\boldsymbol{u},\overset{\star}{\boldsymbol{u}}$ and $\boldsymbol{t},\overset{\star}{\boldsymbol{t}}$ are unknown (resp. known) over the *same* portions of the boundary. Then $(\overset{\star}{\boldsymbol{u}},\overset{\star}{\boldsymbol{t}})$ are linear forms over $\boldsymbol{\theta}$, provided their prescribed parts are themselves linear forms over $\boldsymbol{\theta}$. Also, the second-order rate BIE (49) does not define, for given $\boldsymbol{\theta},\boldsymbol{\mu},\boldsymbol{\chi}$, a unique pair $(\overset{\star\vee}{\boldsymbol{u}},\overset{\star\vee}{\boldsymbol{t}})$.

As a consequence of comments made in †2.3, the first-order rate BIE (35), defined for bodies dependent on a finite number of shape parameters, can indeed be considered as the governing BIE for elastic shape sensitivities in an infinitesimal change of boundary $\boldsymbol{\theta}$, without reference to shape parameters. On the contrary, such interpretation regarding the second-order rate BIE (49) has to be made with much more caution, due to the significant differences between second-order material derivatives and the domain derivative, which we outlined in †2.3.

The pairs $(\boldsymbol{u},\boldsymbol{t})$ in the elastic BIE (19), $(\overset{\star}{\boldsymbol{u}},\overset{\star}{\boldsymbol{t}})$ in the first-order rate BIE (35) and $(\overset{\star\vee}{\boldsymbol{u}},\overset{\star\vee}{\boldsymbol{t}})$ in the second-order rate BIE (49) are governed by the same integral operators. More precisely, if $\boldsymbol{\Phi}(\cdot;\boldsymbol{p})$ is chosen as previously suggested, the components of $(\boldsymbol{u},\boldsymbol{t})$ which are not prescribed by the boundary conditions, those of $(\overset{\star}{\boldsymbol{u}},\overset{\star}{\boldsymbol{t}})$ and those of $(\overset{\star\vee}{\boldsymbol{u}},\overset{\star\vee}{\boldsymbol{t}})$ are governed by the same integral operator. This is of great practical importance, in a computational viewpoint: the discretized integral operator is built and factored in the course of a boundary element solution to (19) and later reused for the numerical solution of the rate BIEs (35), (DRDD). Thus, the complete set of first- and second-order boundary sensitivities is computable by building the right-hand side of (35) for each p_i, i.e. each $\boldsymbol{\theta}$, considered in the first-order case and then of (49) for each pair $(p_i,p_j), i \leq j$, i.e. each $(\boldsymbol{\theta},\boldsymbol{\mu})$, in the second-order case, then solving as many triangular systems as right-hand sides so constructed. Hence it is achievable at an additional computational cost which is reasonable compared to that necessary to solve the elastic BIE.

4 BEM discretization

This section shortly discusses some relevant aspects to the BE discretization of BIEs (19), (35), (49).

4.1 Geometrical modelling in the presence of design variables.

We consider the usual BE discretization of $\partial\Omega$, in which the approximate surface on a given boundary element E is created by interpolation of N nodes $\boldsymbol{y}^k$ $(1 \leq k \leq N)$ (which usually belong to the true boundary) using a mapping of E onto a reference element E_0 (usually the square $\boldsymbol{\xi} = (\xi_1, \xi_2) \in [-1,1]^2$ or the triangle $0 \leq \xi_1 + \xi_2 \leq 1$) and shape functions $N^k(\boldsymbol{\xi})$:

$$\boldsymbol{y} = \sum_{k=1}^{N} N^k(\boldsymbol{\xi})\boldsymbol{y}^k \qquad (\boldsymbol{\xi} \in E_0) \tag{50}$$

Let us also assume an isoparametric discretization for the elastic boundary fields in terms of nodal values $\boldsymbol{u}^k, \boldsymbol{t}^k$:

$$[\boldsymbol{u}, \boldsymbol{t}](\boldsymbol{y}) = \sum_{k=1}^{N} N_k(\boldsymbol{\xi})[\boldsymbol{u}^k, \boldsymbol{t}^k] \qquad (\boldsymbol{\xi} \in E_0) \tag{51}$$

In the presence of a varying boundary (which depends on, say, two parameters p_1, p_2), it is then consistent with the interpolation approach to simply use (50) with nodes following moving according to the geometrical transformation:

$$\boldsymbol{y}^k(\boldsymbol{p}) = \boldsymbol{\Phi}(\boldsymbol{Y}^k; \boldsymbol{p})$$

In this case, considering two generic shape parameters p_1, p_2, the discretized transformation velocities $\boldsymbol{\theta}, \boldsymbol{\mu}, \boldsymbol{\chi}$ associated with (50) admits a BE-type interpolation (51), with nodal values $\boldsymbol{y}^k_{,p_1}, \boldsymbol{y}^k_{,p_2}, \boldsymbol{y}^k_{,p_1p_2}$ respectively. Such interpolation method is consistent with the requirement (32).

4.2 Structure of the discrete linear system.

The discretization of BIEs (19), (35), (49) leads to linear systems of the form:

$$\begin{aligned}
[\boldsymbol{A}]\,\{\boldsymbol{u}\} + [\boldsymbol{B}]\{\boldsymbol{t}\} &= \{\boldsymbol{0}\} \\
[\boldsymbol{A}]\,\{\overset{\star}{\boldsymbol{u}}\} + [\boldsymbol{B}]\{\overset{\star}{\boldsymbol{t}}\} &= \{\boldsymbol{f}^1(\boldsymbol{u}, \boldsymbol{t}; \boldsymbol{\theta})\} \\
[\boldsymbol{A}]\,\{\overset{\star\vee}{\boldsymbol{u}}\} + [\boldsymbol{B}]\{\overset{\star\vee}{\boldsymbol{t}}\} &= \{\boldsymbol{f}^2(\boldsymbol{u}, \boldsymbol{t}, \overset{\star}{\boldsymbol{u}}, \overset{\star}{\boldsymbol{t}}; \boldsymbol{\theta}, \boldsymbol{\mu}, \boldsymbol{\chi})\}
\end{aligned}$$

which, as has been previously noticed, share the same governing (discrete) operators $[\boldsymbol{A}], [\boldsymbol{B}]$. After appropriate column switches, one gets linear systems of equations on the unknown parts $\boldsymbol{v}, \overset{\star}{\boldsymbol{v}}, \overset{\star\vee}{\boldsymbol{v}}$ of the elastostatic state and its sensitivities:

$$\begin{aligned}
[\boldsymbol{K}]\,\{\boldsymbol{v}\} &= \{\boldsymbol{g}^0\} \\
[\boldsymbol{K}]\,\{\overset{\star}{\boldsymbol{v}}\} &= \{\boldsymbol{g}^1(\boldsymbol{v}; \boldsymbol{\theta})\} \\
[\boldsymbol{K}]\,\{\overset{\star\vee}{\boldsymbol{v}}\} &= \{\boldsymbol{g}^2(\boldsymbol{v}, \overset{\star}{\boldsymbol{v}}; \boldsymbol{\theta}, \boldsymbol{\mu}, \boldsymbol{\chi})\}
\end{aligned}$$

These systems are governed by the same (discrete) operator $[\boldsymbol{K}]$. However for this to be true the analytical description of the geometric transformation must be chosen so as the Dirichlet and Neumann parts of $\partial\Omega$ are material surfaces.

4.3 Discretization of tangential differential operators

The first- and second-order rate BIEs (35), (49) make use of various tangential differential operators, for which BE implementation-oriented expressions are given below. First, the natural basis $(\boldsymbol{a}_\alpha)$, metric tensor $(g_{\alpha\beta})$, jacobian $J(\boldsymbol{\xi})$ and unit normal $\boldsymbol{n}$ on E associated with interpolation (50) are given by:

$$\boldsymbol{a}_\alpha(\boldsymbol{\xi}) = \sum_{k=1}^{N} N^k_{,\alpha}(\boldsymbol{\xi})\boldsymbol{y}^k \qquad g_{\alpha\beta}(\boldsymbol{\xi}) = \boldsymbol{a}_\alpha(\boldsymbol{\xi}) \cdot \boldsymbol{a}_\beta(\boldsymbol{\xi})$$
$$\mathrm{d}S = J(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi} = [(g_{11}g_{22} - g_{12}^2)(\boldsymbol{\xi})]^{1/2}\,\mathrm{d}\boldsymbol{\xi} \qquad J(\boldsymbol{\xi})\boldsymbol{n}(\boldsymbol{\xi}) = \boldsymbol{a_1} \wedge \boldsymbol{a_2}$$

Then from classical differential geometry the surface gradient $\boldsymbol{\nabla}_S f$ of a scalar function expressed in terms of the variable $\boldsymbol{\xi} \in E_0$ is given by:

$$\boldsymbol{\nabla}_S f = (D_r f)\boldsymbol{e}_r \qquad \text{with} \quad D_r f = f_{,\alpha} g^{\alpha\beta}(\boldsymbol{a_\beta}.\boldsymbol{e_r}) \qquad (f_{,\alpha} \equiv \frac{\partial f}{\partial \xi_\alpha}) \tag{52}$$

using the contravariant representation of $\boldsymbol{g}$, i.e. $g^{\alpha\gamma}g_{\gamma\beta} = \delta^\alpha_\beta$. This also holds for the components of vector or tensor fields, provided they are expressed in cartesian coordinates. One can then establish from (52) the following formulae:

$$D_r u_r = u_{r,\alpha} g^{\alpha\beta}(\boldsymbol{a_\beta}.\boldsymbol{e_r}) \tag{53}$$
$$D_{rj} f\,\mathrm{d}S_y = \epsilon_{irj}\,[f_{,1}(\boldsymbol{a_2}.\boldsymbol{e_i}) - f_{,2}(\boldsymbol{a_1}.\boldsymbol{e_i})]\,\mathrm{d}\boldsymbol{\xi} \tag{54}$$

Eqns. (52-53-54) allow the discretisation of surface divergence and other tangential differential operators which appear in the BIEs (35) and (49).

4.4 Numerical evaluation of singular integrals in RDBIE

Singular integrals occur if E contains the collocation point $\boldsymbol{x}$. A typical singular integral appearing in (49) is:

$$I^s = \int_E [\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})][\mu_q(\boldsymbol{y}) - \mu_q(\boldsymbol{x})]\Sigma^k_{ij,q}(\boldsymbol{x},\boldsymbol{y}) D_{rj} u_i\,\mathrm{d}S_y \tag{55}$$

Let $\boldsymbol{\eta} = (\eta_1, \eta_2)$ denote the antecedent of $\boldsymbol{x}$ on E_0. For any usual shape function $N(\boldsymbol{\xi})$, one can define auxiliary functions N^I_α such that:

$$N(\boldsymbol{\xi}) = N(\boldsymbol{\eta}) + (\xi_\alpha - \eta_\alpha)N^I_\alpha(\boldsymbol{\xi};\boldsymbol{\eta}) \tag{56}$$

Following a common practice in BEM (see e.g. [17]), set $\xi_1 = \rho\cos\alpha$, $\xi_2 = \rho\sin\alpha$. Then $\mathrm{d}\boldsymbol{\xi} = \rho d\rho d\alpha$ and, from (56):

$$N(\boldsymbol{\xi}) - N(\boldsymbol{\eta}) = \rho\hat{M}^q(\rho,\alpha;\boldsymbol{\eta}) \quad \text{with} \quad \hat{M}^q(\rho,\alpha;\boldsymbol{\eta}) = \cos\alpha N^I_1(\boldsymbol{\xi};\boldsymbol{\eta}) + \sin\alpha N^I_2(\boldsymbol{\xi};\boldsymbol{\eta}) \tag{57}$$

so that one has from (50):

$$r = \| \boldsymbol{x} - \boldsymbol{y} \| = \| \sum_{k=1}^{N} \rho \hat{N}^k(\rho, \alpha; \boldsymbol{\eta}) \boldsymbol{y}^k \| \equiv \rho \hat{r}(\rho, \alpha; \boldsymbol{\eta}) \tag{58}$$

where $\hat{r}(\rho, \alpha; \boldsymbol{\eta}) \neq 0$. Consequently, since the derivatives of $\Sigma^k(\boldsymbol{x}, \boldsymbol{y})$ behave like r^{-3}:

$$\Sigma^k_{ij,q}(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{\rho^3} \hat{\Sigma}^k_{ij,q}(\rho, \alpha; \boldsymbol{\eta}) \tag{59}$$

where $\hat{r}(\rho, \alpha; \boldsymbol{\eta}) \neq 0$ and $\hat{\Sigma}^k_{ij,q}(\rho, \alpha; \boldsymbol{\eta})$ is regular at $\rho = 0$. Also, from (51), one can put

$$\boldsymbol{\theta}(\boldsymbol{y}) - \boldsymbol{\theta}(\boldsymbol{x}) = \rho \sum_{k=1}^{N} \boldsymbol{y}^k_{,p_1} \hat{N}^k(\rho, \alpha; \boldsymbol{\eta}) \tag{60}$$

and similar expressions for $[\boldsymbol{\mu}(\boldsymbol{y}) - \boldsymbol{\mu}(\boldsymbol{x})]_{,\ldots}$ Using these definitions, integral (55) is recast in a completely regular form as:

$$I^s = \sum_{k=1}^{N} \sum_{\ell=1}^{N} y^k_{r,p_1} y^\ell_{q,p_2} \int_E \hat{N}^k(\rho, \alpha; \boldsymbol{\eta}) \hat{N}^\ell(\rho, \alpha; \boldsymbol{\eta}) \hat{\Sigma}^k_{ij,q}(\rho, \alpha; \boldsymbol{\eta}) D_{rj} u_i J(\boldsymbol{\xi}) d\rho d\alpha \tag{61}$$

where the discretization of $D_{rj}u_i$ is not shown for brevity. Expression (61) takes full advantage of the regularization; its numerical evaluation of (61) can be performed with standard product Gaussian quadrature formulas, the complete procedure requiring a further coordinate change $(\rho, \alpha) \to (v_1, v_2)$ in order to recover an integral over the square $[-1, 1]^2$.

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A Appendix

A.1 Proof of identity (42)

It relies on a series of integrations by parts. First, the classical divergence-flux formula gives:

$$\int_{\partial\Omega} A_{ij}(\boldsymbol{y})n_j(\boldsymbol{y})U_i^k(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}S_y = \int_{\Omega} U_i^k(\boldsymbol{x},\boldsymbol{y})A_{ij,j}(\boldsymbol{y})\,\mathrm{d}V_y + \int_{\Omega} U_{i,j}^k(\boldsymbol{x},\boldsymbol{y})A_{ij}(\boldsymbol{y})\,\mathrm{d}V_y \tag{62}$$

Now, using the definition (39) of $\boldsymbol{A}$, the second integral above reads:

$$\begin{aligned} I &= \int_{\Omega} U_{i,j}^k \left\{C_{ijpq}(u_{p,r}\theta_{r,q} - u_{p,q}\theta_{r,r}) + \sigma_{ir}\theta_{jr}\right\}\,\mathrm{d}V \\ &= \int_{\Omega} \left\{\Sigma_{ij}^k(u_{i,r}\theta_{r,j} - u_{i,j}\theta_{r,r}) + U_{i,j}^k\sigma_{ir}\theta_{s,r}\right\}\,\mathrm{d}V \end{aligned} \tag{63}$$

(the arguments $\boldsymbol{x},\boldsymbol{y}$ being omitted for brevity). Next, one notes the following consequence of the classical divergence-flux formula:

$$\int_{\Omega}(fg_{,r}h_{,j} - fg_{,j}h_{,r})\,\mathrm{d}V = \int_{\Omega}(gh_{,r}f_{,j} - gh_{,j}f_{,r})\,\mathrm{d}V + \int_{\partial\Omega} fgD_{rj}h\,\mathrm{d}S$$

which gives, noting for regularisation purposes that $\theta_{r,j}(\boldsymbol{y}) = [\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})]_{,j}$ holds:

$$\begin{aligned} &\int_{\Omega} \Sigma_{ij}^k(u_{i,r}\theta_{r,j} - u_{i,j}\theta_{r,r})\,\mathrm{d}V \\ &= -\int_{\partial\Omega} D_{rj}u_i[\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})]\Sigma_{ij}^k\,\mathrm{d}S + \int_{\Omega}[\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})]\left\{\Sigma_{ij,r}^k u_{i,j} - \Sigma_{ij,j}^k u_{i,r}\right\}\,\mathrm{d}V \\ &= -\int_{\partial\Omega} D_{rj}u_i[\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})]\Sigma_{ij}^k\,\mathrm{d}S + \int_{\Omega}[\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})]\Sigma_{ij,r}^k u_{i,j}\,\mathrm{d}V \end{aligned} \tag{64}$$

where use has been made of the equilibrium equation $\Sigma_{ij,j}^k = 0$ ($\boldsymbol{y} \neq \boldsymbol{x}$). Besides, one notes that:

$$\begin{aligned} \int_{\Omega} U_{i,j}^k\sigma_{ir}\theta_{s,r}\,\mathrm{d}V &= \int_{\partial\Omega} U_{i,j}^k[\theta_j(\boldsymbol{y}) - \theta_j(\boldsymbol{x})]\sigma_{ir}n_r\,\mathrm{d}S - \int_{\Omega} U_{i,rj}^k\sigma_{ir}[\theta_j(\boldsymbol{y}) - \theta_j(\boldsymbol{x})]\,\mathrm{d}V \\ &= \int_{\partial\Omega} U_{i,j}^k[\theta_j(\boldsymbol{y}) - \theta_j(\boldsymbol{x})]t_i\theta_j\,\mathrm{d}S - \int_{\Omega} \Sigma_{ir,j}^k u_{i,r}[\theta_j(\boldsymbol{y}) - \theta_j(\boldsymbol{x})]\,\mathrm{d}V \end{aligned} \tag{65}$$

Finally, eqns. (64-65) imply that the integral I (63) can be expressed as:

$$I = \int_{\partial\Omega} t_i(\boldsymbol{y})[\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})]U_{i,r}^k(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}S_y - \int_{\partial\Omega}[\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})\Sigma_{ij}^k(\boldsymbol{x},\boldsymbol{y})D_{rj}u_i(\boldsymbol{y})\,\mathrm{d}S_y$$

which, in view of (62), finally proves the identity (42).

A.2 Expressions for $\overset{\star}{\widehat{D_{rj}u_i}}$, $\overset{\star}{\widehat{D_r u_i}}$, $\overset{\star}{\widehat{D_r\theta_r}}$

Starting from the definition

$$D_{rj}u_i = n_r u_{i,j} - n_j u_{i,r}$$

and using equations (4), (9), one has:

$$\begin{aligned}
\widehat{D_{rj}u_i}^{\star} &= n_r(\overset{\star}{u}_{i,j} - u_{i,q}\theta_{q,j}) - n_q D_r\theta_q u_{i,j} - n_s(\overset{\star}{u}_{i,r} - u_{i,q}\theta_{q,r}) + n_q D_j\theta_q u_{i,r} \\
&= D_{rj}\overset{\star}{u}_i - u_{i,q}D_{rj}\theta_q + n_q D_j\theta_q u_{i,r} - n_q D_r\theta_q u_{i,j} \\
&= D_{rj}\overset{\star}{u}_i - u_{i,q}D_{rj}\theta_q + u_{i,q}D_{rj}\theta_q + D_j\theta_q D_{qr}u_i + D_r\theta_q D_{sq}u_i \\
&= D_{rj}\overset{\star}{u}_i + D_j\theta_q D_{qr}u_i + D_r\theta_q D_{sq}u_i
\end{aligned} \tag{66}$$

Next, one notes that:

$$-n_j D_{rj}u_i = n_j(n_j D_r u_i - n_r D_r u_i) = D_r u_i$$

since $\boldsymbol{n}.\boldsymbol{\nabla}_S\boldsymbol{u} = \boldsymbol{0}$ by virtue of definition (7). Hence, one can combine eqns. (9) and (66) to get:

$$\begin{aligned}
\widehat{D_r u_i}^{\star} &= -n_j\,\widehat{D_{rj}u_i}^{\star} - \overset{\star}{n}_j\,D_{rj}u_i \\
&= -n_j\,\widehat{D_{rj}u_i}^{\star} + n_q D_j\theta_q D_{rj}u_i \\
&= D_r\overset{\star}{u}_i - D_r\theta_q D_q u_i + n_q D_j\theta_q D_{rj}u_i
\end{aligned} \tag{67}$$

Finally, the above formula with $\boldsymbol{u} = \boldsymbol{\theta}$, $i = r$ and summation over r yields (note that $\overset{\vee}{\boldsymbol{\theta}} = \boldsymbol{\chi}$):

$$\widehat{\mathrm{div}_S\boldsymbol{\theta}}^{\star} = \mathrm{div}_S\boldsymbol{\chi} - \boldsymbol{\nabla}_S\boldsymbol{\theta} : \boldsymbol{\nabla}_S\boldsymbol{\mu} + \overset{\star}{\boldsymbol{n}}\,.\,\overset{\vee}{\boldsymbol{n}} \tag{68}$$

A.3 Proof of the symmetry of $K_1(\boldsymbol{x}, \boldsymbol{u}; \boldsymbol{\theta}, \boldsymbol{\mu})$

It rests on the fact that $J_1(\boldsymbol{x}, \boldsymbol{u}; \boldsymbol{\theta})$ admits the alternative expression (30):

$$J_1(\boldsymbol{x}, \boldsymbol{u}; \boldsymbol{\theta}) = \int_{\partial\Omega} [u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})]\left\{[\theta_r(\boldsymbol{y}) - \theta_r(\boldsymbol{x})]n_j(\boldsymbol{y})\Sigma^k_{ij,r}(\boldsymbol{x},\boldsymbol{y}) - D_{rj}\theta_r(\boldsymbol{y})\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y})\right\}\,\mathrm{d}S_y$$

which was the one obtained before integration by parts. Then one may take the material derivative of I_1 by applying (10) to the above expression instead of (34). On account of identities (9), (28), one has:

$$\begin{aligned}
\overset{\vee}{J}_1(\boldsymbol{x}, \boldsymbol{u}; \boldsymbol{\theta}) &= \int_{\partial\Omega} [\overset{\vee}{u}_i(\boldsymbol{y}) - \overset{\vee}{u}_i(\boldsymbol{x})]\left\{n_j(\boldsymbol{y})\,\overset{\star}{\Sigma}{}^k_{ij}(\boldsymbol{x},\boldsymbol{y}) - D_{rj}\theta_r(\boldsymbol{y})\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y})\right\}\mathrm{d}S_y \\
&+ \int_{\partial\Omega} [u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})]\{[\chi_r(\boldsymbol{y}) - \chi_r(\boldsymbol{x})]n_j(\boldsymbol{y})\Sigma^k_{ij,r}(\boldsymbol{x},\boldsymbol{y}) - \overset{\vee}{\widehat{D_{rj}\theta_r}}(\boldsymbol{y})\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y})\}\,\mathrm{d}S_y \\
&+ \int_{\partial\Omega} [u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})]\left\{n_j(\boldsymbol{y})\,\overset{\star\vee}{\Sigma}{}^k_{ij}(\boldsymbol{x},\boldsymbol{y}) + \overset{\star}{\Sigma}{}^k_{ij}(\boldsymbol{x},\boldsymbol{y})D_{sq}\mu_q(\boldsymbol{y}) - \overset{\vee}{\Sigma}{}^k_{ij}(\boldsymbol{x},\boldsymbol{y})D_{qj}\theta_q(\boldsymbol{y})\right\}\mathrm{d}S_y \\
&- \int_{\partial\Omega} [u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})]\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y})D_{rj}\theta_r(\boldsymbol{y})D_q\mu_q(\boldsymbol{y})\,\mathrm{d}S_y
\end{aligned}$$

which, using expression (66) for $\widehat{D_{rj}u_i}^{\star}$ and upon some algebraic manipulations, leads to the following result:

$$\overset{\vee}{J}_1(\boldsymbol{x}, \boldsymbol{u}; \boldsymbol{\theta}) = J_1(\boldsymbol{x}, \boldsymbol{u}; \boldsymbol{\chi}) + J_1(\boldsymbol{x}, \overset{\vee}{\boldsymbol{u}}; \boldsymbol{\theta}) + K_1(\boldsymbol{x}, \boldsymbol{u}; \boldsymbol{\theta}, \boldsymbol{\mu})$$

where

$$\begin{aligned}
K_1(\boldsymbol{x}, \boldsymbol{u}; \boldsymbol{\theta}, \boldsymbol{\mu}) &= \int_{\partial\Omega} [u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})]\left\{n_j(\boldsymbol{y})\,\overset{\star\vee}{\Sigma}{}^k_{ij}(\boldsymbol{x},\boldsymbol{y}) + \overset{\star}{\Sigma}{}^k_{ij}(\boldsymbol{x},\boldsymbol{y})D_{sq}\mu_q(\boldsymbol{y}) + \overset{\vee}{\Sigma}{}^k_{ij}(\boldsymbol{x},\boldsymbol{y})D_{sq}\theta_q(\boldsymbol{y})\right\}\mathrm{d}S_y \\
&\quad - \int_{\partial\Omega} [u_i(\boldsymbol{y}) - u_i(\boldsymbol{x})]\Sigma^k_{ij}(\boldsymbol{x},\boldsymbol{y})d_j(\boldsymbol{y})\,\mathrm{d}S_y
\end{aligned}$$

and

$$d_j = n_r \left(D_j\theta_r D_q\mu_q + D_j\mu_r D_q\theta_q - D_j\mu_q D_q\theta_r - D_j\theta_q D_q\mu_r\right) + n_j \left(D_q\theta_r D_r\mu_q - D_r\theta_r D_q\mu_q\right)$$

in which the symmetry of K_1 with respect to $(\boldsymbol{\theta}, \boldsymbol{\mu})$ is now apparent. It is however preferable to use the earlier, more compact, expression (48) of $\check{J}_1$, for practical purposes.